THE PHYSICS OF SUBGRID SCALES IN NUMERICAL SIMULATIONS OF STELLAR CONVECTION: ARE THEY DISSIPATIVE, ADVECTIVE, OR DIFFUSIVE?

V. M. CANUTO

NASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY 10025; and Department of Applied Physics,
Columbia University, New York, NY 10027

ABSTRACT

All numerical simulations of stellar convection assume that the unresolved subgrid scales (SGSs) are only dissipative. We show that the assumption is incorrect and that the SGSs *stir* (advection), *mix* (diffusion), and *dissipate*. The first two processes were never considered before. We also show that there are two advective velocities: one contributed by the resolved scales and the other, a *bolus velocity*, by the unresolved scales.

Subject headings: convection — stars: evolution — stars: interiors

1. THE PROBLEM

Large-eddy simulation (LES) is a technique that attempts to solve numerically the exact energy and momentum equations. What fraction of the total number of scales are numerically resolved? The ratio of the largest L to the smallest l scales and the number of grid points N to be resolved is given by (the Sun Re is $\approx 10^{12}$)

$$\frac{L}{l} \sim \mathrm{Re}^{3/4} \sim 10^9, \quad N \sim \left(\frac{L}{l}\right)^3 \sim \mathrm{Re}^{9/4} \sim 10^{27},$$

$$N_{\max} \sim 10^{12}. \qquad (1a)$$

The maximum $N_{\max}$ attainable with today's computers is some 15 orders of magnitude short of what is required to numerically resolve all the dynamic scales of the problem. Alternatively, LESs resolve not even 1% of the number of scales given by the first equation (1a). Thus, the subgrid scales (SGSs) must contain very large scales and of course medium and small scales. How have the large and small SGSs been represented? All LESs have assumed without proof that the SGSs are purely dissipative (Sofia & Chan 1984; Xie & Toomre 1991; Hossain & Mullan 1991; Porter & Woodward 1994; Stein & Nordlund 1998; Kim & Chan 1998, hereafter KC). However, a simple argument shows that the assumption cannot be correct. Dissipation is a small-scale process, while the SGSs still contain large scales that can also stir (advect) and mix (diffuse). The often-cited argument that variations of the constants in the dissipation-only SGS model do not alter the LES results is inadequate; if a model does not contain some basic physics, no variation of the constants can resurrect what is not there. What about mixing? Mixing is a diffusive process that still cannot fully represent the large unresolved scales. What about stirring? Stirring, often also called folding and/or streaking, is an advective process that can occur even in the absence of mixing and even if the motion is not turbulent. Kneading the dough is the simplest example. Thus, to properly represent both large and small SGSs, one needs

$$\text{stirring (advection), mixing (diffusion), dissipation.} \quad (1b)$$

2. MOMENTUM AND TEMPERATURE MEAN EQUATIONS

We write the exact dynamic equation for the resolved (denoted by an overbar) momentum and temperature fields as they are written in most LES calculations, namely,

$$\bar{\rho} \frac{D}{Dt} \bar{u}_i = -\frac{\partial}{\partial x_j} (\bar{p}\delta_{ij} + \bar{\rho}\tau_{ij}) - \bar{\rho}g_i, \qquad (2a)$$

$$c_v \bar{\rho} \frac{D\overline{T}}{Dt} = -\bar{p}\frac{\partial \bar{u}_i}{\partial x_i} + \bar{\rho}Q(\mathrm{rad}) + \bar{\rho}Q(\mathrm{vis}), \qquad (2b)$$

where $D/Dt \equiv \partial/\partial t + \bar{u}_i \partial/\partial x_i$. The SGSs are represented by the Reynolds stresses τ_{ij} (u_i' is the unresolved component of the velocity field),

$$\tau_{ij} = \bar{\rho}^{-1}\langle \rho u_i' u_j' \rangle, \qquad (2c)$$

and by $Q(\mathrm{vis})$. To obtain $Q(\mathrm{vis})$, we compare equation (2b) with the exact temperature equation derived in equation (20h) of Canuto (1997, hereafter C97). The result is

$$Q(\mathrm{vis}) = -\tau_{ij}\bar{s}_{ij} - \bar{u}_i \frac{\partial K}{\partial x_i} - \bar{\rho}^{-1}\frac{\partial}{\partial x_i}(F_i^c + F_i^{\kappa e}) - \frac{\partial K}{\partial t}, \quad (2d)$$

where $2\bar{s}_{ij} = \bar{u}_{i,j} + \bar{u}_{j,i}$ is the shear generated by the resolved scales, K is the kinetic energy $K = \frac{1}{2}\tau_{ii}$, $\boldsymbol{F}^c$ is the convective flux, and $\boldsymbol{F}^{\kappa e}$ is the flux of kinetic energy:

$$\boldsymbol{F}^c = c_p \langle \rho \boldsymbol{u}' T' \rangle, \quad \boldsymbol{F}^{\kappa e} = \frac{1}{2}\langle \rho u_i' u_i' \boldsymbol{u}' \rangle. \qquad (2e)$$

Equations (2a)–(2e) are exact. In equation (2d), the first term represents a local source of thermal energy $c_v T$ since $-\tau_{ij}\bar{s}_{ij} > 0$. The origin of this source is readily identified. Viscous forces cause a loss of kinetic energy, which, by energy conservation, becomes a source of thermal energy (the generally used characterization "viscous" in $Q(\mathrm{vis})$ is thus inappropriate). The second term represents *advection* of SGS kinetic energy gradients by the resolved fields $\bar{\boldsymbol{u}}$. The second and third terms represent both *diffusion* and advection by a "bolus velocity," as we shall show. The time derivative of K makes the model dynamical. Thus, the physical arguments leading to equation (1b) are confirmed by the exact equations.

3. PREVIOUS SGS MODELS

Thus far, all LESs have assumed that the SGSs are purely dissipative, which means that

$$Q(\text{vis}) = -\tau_{ij}\bar{s}_{ij} = \epsilon, \qquad (3)$$

where the last step comes from assuming that $P = \epsilon$, where $P = -\tau_{ij}\bar{s}_{ij}$ is the production. How is ϵ computed? By definition,

$$\bar{\rho}\epsilon = \langle \sigma_{ij}u_{i,j}\rangle, \quad \sigma_{ij} = \nu\rho(u_{i,j} + u_{j,i}) - \frac{2}{3}\nu\rho\delta_{ij}u_{k,k}, \quad (4a)$$

where σ_{ij} is the viscous stress tensor, $u_i = \bar{u}_i + u_i'$ is the total velocity field (resolved and unresolved components), and ν is the kinematic viscosity. One further has

$$\bar{\rho}\epsilon = \langle \sigma_{ij}u_{i,j}\rangle = \sigma_{ij}(\bar{u})\bar{u}_{i,j} + \langle \sigma_{ij}'u_{i,j}'\rangle, \qquad (4b)$$

and since the large scales have a lifetime much longer than small scales,

$$\langle \sigma_{ij}'u_{i,j}'\rangle \gg \sigma_{ij}(\bar{u})\bar{u}_{i,j}, \qquad (4c)$$

one finally has

$$Q(\text{vis}) = \epsilon = \bar{\rho}^{-1}\langle \sigma_{ij}'u_{i,j}'\rangle. \qquad (4d)$$

There are two models to compute ϵ. In k-space, equation (4d) becomes

$$\epsilon = 2\nu \int k^2 E(k)dk, \qquad (4e)$$

and if one knew the turbulent energy spectrum $E(k)$, one could in principle use equation (4e). In stars, the very low value of ν makes the use of equation (4e) very problematic, for one needs a detailed knowledge of $E(k)$ at very high values of k, something we do not have. Thus, equation (4e) is of little practical use. Thus, one must solve the dynamic equation for ϵ (C97, eq. [28a]):

$$\frac{D\epsilon}{Dt} + \frac{\partial}{\partial x_i}F_i(\epsilon) = (c_s\bar{\rho}P - c_1 g_i\langle \rho'u_i'\rangle)\epsilon K^{-1} - c_2\epsilon^2 K^{-1}, \quad (5a)$$

where $F(\epsilon)$ is the flux of ϵ given by

$$F_i(\epsilon) = -\nu_t \frac{\partial \epsilon}{\partial x_i}. \qquad (5b)$$

No astrophysical LES has ever used equations (5a) and (5b). Rather, they compute ϵ in a peculiar way. They actually "invert" equation (4c), and instead of equation (4d) they take

$$Q(\text{vis}) = \epsilon = \bar{\rho}^{-1}\sigma_{ij}(\nu = \nu_*, \bar{u})\bar{u}_{i,j}, \qquad (5c)$$

where ν_* is some "invented" viscosity. Not only is the process of turning equation (4c) on its head physically unappealing, but the final result (eq. [5c]), a Pyrrhic victory for the advantage of having made the fluctuating fields in equation (4d) disappear in favor of the known resolved fields $\bar{u}$ in equation (5c), has

a high cost, the unknown ν_*, the evaluation of which being quite a problem.

Hyperviscosity models.—These models entail derivatives higher than the Laplacian and are merely a numerical device to help the numerics. Gille & Davis (1999) have shown that they have a "skill index" Z of only 10% (Z is defined as the percentage of the mean squared SGS flux produced by a given model vis-à-vis the one computed with an eddy resolving model). The hyperviscosity model has the poorest performance of all SGSs.

Numerical viscosity models.—In some LESs, ν_* is adjusted to ensure numerical stability, but Marcus (1986) has shown that this alters the nature of the flow from an inviscid turbulent flow to a laminar, viscous flow, thus altering the true nature of the problem.

KC model.— KC adopted equation (5c) but avoided the use of a numerical ν_*. Instead, they adopt the Smagorinsky-Lilly model (SLM):

$$\nu_* = (C\Delta)^2\Sigma, \quad \Sigma = (2\bar{s}_{ij}\bar{s}_{ij})^{1/2}, \quad \pi C = \left(\frac{2}{3\text{Ko}}\right)^{3/4}, \quad (6a)$$

$$\tau_{ij} = -2\nu_*\bar{s}_{ij} + \frac{2}{3}K\delta_{ij}, \quad K = \pi^{-2}\Sigma^2\Delta^2, \quad \epsilon = (C\Delta)^2\Sigma^3. \quad (6b)$$

Here Δ is the size of the smallest resolved eddy and Ko $\sim$ 1.6 is the Kolmogorov constant. The SGS model is thus expressed in terms of the resolved scales only. Although the KC model improves the evaluation of ν_*, several shortcomings must be pointed out:

1. The KC model is only dissipative.
2. Equations (6a) and (6b) are valid for incompressible flows and underestimate ϵ. In C97 it was shown that in the compressible case, ϵ has two contributions: a solenoidal, incompressible part $\epsilon(s)$ given by equation (5a) and a dilatation compressible part $\epsilon(d)$; $\epsilon = \epsilon(s) + \epsilon(d)$. A useful parameterization (C97) is

$$\epsilon = \epsilon(s)[1 + F(M)], \quad M^2 = 2K(\gamma RT)^{-1}, \qquad (6c)$$

with $F(x) = \alpha_1 x^2$, $\alpha_1 \approx 1$. The result is that *compressibility increases dissipation.*

3. Kimmel & Domaradzki (2000) have shown that the SLM fails to predict the shape of the subgrid stresses τ_{ij} qualitatively and severely underestimates the largest value. Their conclusion is that the SLM poorly represents the actual SGS processes.

4. Equation (6b) assumes that the SGS Reynolds stresses τ_{ij} are "aligned" with the large-scale shear $\bar{s}_{ij}$, an unlikely assumption (Canuto 1994) that Kimmel & Domaradzki (2000) have given further reasons to doubt. In addition, τ_{ij} lacks the contribution of buoyancy.

4. CONSISTENCY TEST

Even if one decides to adopt the incomplete dissipation-only model (eq. [5c]), ν_* must be chosen to satisfy the requirement (ϵ is given by eqs. [5a], [5b], and [6c])

$$\nu_* = \epsilon(\Sigma_{ij}\bar{u}_{i,j})^{-1}, \quad \Sigma_{ij} = (\bar{u}_{i,j} + \bar{u}_{j,i}) - \frac{2}{3}\delta_{ij}\bar{u}_{k,k}. \qquad (7)$$

This is the *consistency test* that LESs with a dissipation-only model must satisfy.

5. COMPLETE SGS MODEL

We now provide the relations necessary to compute the full SGS model (§ 9 in Canuto 1999, hereafter C99): Reynolds stresses τ_{ij},

$$\tau_{ij} = -2\nu_t \bar{s}_{ij} + \frac{1}{5}\frac{K}{\epsilon}B_{ij} + \frac{2}{3}K\delta_{ij}, \qquad (8a)$$

$$\nu_t = \frac{8}{75}\frac{K^2}{\epsilon}, \quad B_{ij} = \alpha\left(g_i J_j + g_j J_i - \frac{2}{3}\delta_{ij}g_k J_k\right). \qquad (8b)$$

Equation (8a) contains the contribution of buoyancy, as required by the Navier-Stokes equations. Heat flux $\boldsymbol{F}^c = c_p\bar{\rho}\boldsymbol{J}$;

$$(\delta_{ij} + \mu_{ij})J_j = \chi_t K^{-1}\tau_{ij}\beta_j. \qquad (8c)$$

Here β_i is the superadiabatic temperature gradient and χ_t is the heat turbulent diffusivity

$$\beta_i = -\frac{\partial T}{\partial x_i} + \left(\frac{\partial T}{\partial x_i}\right)_{\mathrm{ad}}, \quad \chi_t = \sigma_t^{-1}\nu_t, \quad \sigma_t = \frac{\nu_t}{\chi_t} = 0.67. \qquad (8d)$$

The tensor μ_{ij} is given by [$a = 0.16$, $b = 0.215$, and $\lambda_i = -(g\bar{\rho})^{-1}P_i$]:

$$\mu_{ij} = aK\epsilon^{-1}(\bar{s}_{ij} + \bar{v}_{ij}) - bK^2\epsilon^{-2}g\alpha\lambda_i\beta_j, \qquad (8e)$$

where $2\bar{v}_{ij} = (\bar{u}_{i,j} - \bar{u}_{j,i})$ is the vorticity of the resolved scales. Equations (8a)–(8c) are a system of linear equations that can be easily solved. The standard model

$$J_i = \chi_*\beta_i, \quad \chi_* = \frac{2}{3}\chi_t \qquad (9)$$

is a poor approximation of equation (8c); it arbitrarily neglects μ_{ij} and for τ_{ij} takes only the last term in equation (8a). Equation (8c) then becomes equation (9). We suggest not to use equation (9) but equations (8c)–(8e).

6. EQUATIONS FOR K AND ϵ

The above SGS model requires two turbulence variables, K and ϵ. The latter is given by equations (5a) and (6c). For K, one can use three models of increasing complexity. (1) One can use Kolmogorov's model,

$$K = \frac{3\mathrm{Ko}}{2}\left(\frac{\epsilon\Delta}{\pi}\right)^{2/3}. \qquad (10a)$$

(2) One can use a more complete model in which production

is equal to dissipation (eq. [35c] in C97),

$$\epsilon = P - g_i\rho^{-1}\overline{\rho'u_i'}, \quad \overline{\rho'u_i''} = m(\gamma - 1)\bar{\rho}c_p c_s^{-2}J_i, \qquad (10b)$$

and where (C99, eq. [145b])

$$P = -\tau_{ij}\bar{s}_{ij}$$
$$= \nu_t\Sigma^2 - \frac{2}{3}K\left(1 - \frac{1}{5}\epsilon^{-1}\alpha g_i J_i\right)\bar{s}_{kk} - \frac{2}{5}\epsilon^{-1}g\alpha KJ_i\bar{s}_{3i}. \qquad (10c)$$

In equation (10b), c_s is the sound speed, m is a polytropic index ($= -1$ in the Boussinesq approximation), and α is the volume expansion coefficient ($= T^{-1}$ for a perfect gas). (3) One can solve the full dynamic equation for K given by equation (15b) of C97.

7. BOLUS VELOCITY

The new SGS model contains an interesting new physical feature. The third term in equation (2d) seems superficially a diffusion term, but it also contains an advective part that was not uncovered thus far for reasons that will soon become clear. Using the Cayley-Hamilton theorem, equation (8c) can be solved to give ($f_i \equiv \chi_t K^{-1}\tau_{ij}\beta_j$; see the Appendix)

$$J_i = (\Lambda_0\delta_{ij} + \Lambda_1\mu_{ij} + \Lambda_2\mu_{ik}\mu_{kj})f_j. \qquad (11a)$$

We now divide μ_{ij}, equation (8e), into symmetric and antisymmetric parts:

$$\mu_{ij} = \mu_{ij}^S + \mu_{ij}^a, \qquad (11b)$$

where ($\mu_0 \equiv aK\epsilon^{-1}$, $\mu_1 \equiv -bK^2\epsilon^{-2}g\alpha$)

$$\mu_{ij}^s = \mu_0\bar{s}_{ij} + \frac{1}{2}\mu_1(\lambda_i\beta_j + \lambda_j\beta_i), \qquad (11c)$$

$$\mu_{ij}^a = \frac{1}{2}\mu_1(\lambda_i\beta_j - \lambda_j\beta_i) + aK\epsilon^{-1}\bar{v}_{ij}. \qquad (11d)$$

Inserting equation (11b) into equation (11a), we can write, in general,

$$J_i = (K_{ij}^s + K_{ij}^a)\beta_j. \qquad (12)$$

For the present argument we do not need the explicit form of the tensorial diffusivities K_{ij}, which can be easily constructed. The relevant point is that we have both symmetric and antisymmetric K_{ij}'s. Let us now return to the SGS form (eq. [2d]) and concentrate on the third term, which, after using equation

(12), gives rise to

$$\frac{\partial}{\partial x_i}(\bar{\rho} J_i) = \frac{\partial}{\partial x_i}\bar{\rho}(K_{ij}^s + K_{ij}^a)\beta_j. \tag{13a}$$

Next, we rewrite the antisymmetric term as

$$\frac{\partial}{\partial x_i}\bar{\rho} K_{ij}^a \beta_j = \bar{\rho} K_{ij}^a \frac{\partial}{\partial x_i}\beta_j - \bar{\rho} u_j^* \beta_j, \tag{13b}$$

where u_j^* is a bolus velocity, defined as

$$\bar{\rho} u_j^* = -\frac{\partial}{\partial x_i}(\bar{\rho} K_{ij}^a), \tag{13c}$$

which has zero divergence thanks to the antisymmetry of K_{ij}^a;

$$\frac{\partial}{\partial x_i}\bar{\rho} u_i^* = -\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\bar{\rho} K_{ij}^a = 0. \tag{13d}$$

Moving the bolus velocity to the left-hand side of equation (2b), we see that there are two advective terms:

$$c_v \frac{\partial \bar{T}}{\partial t} + (c_v \bar{u}_i + c_p u_i^*)\frac{\partial T}{\partial x_i} = -\bar{\rho}^{-1}\bar{p}\frac{\partial \bar{u}_i}{\partial x_i} + Q(\text{rad}) + \dots . \tag{14}$$

The first is provided by the resolved scales velocity $\bar{u}$, and the second is provided by the bolus velocity u^*, which is due to the unresolved scales. Since the standard model (eq. [9]) neglects μ_{ij}, the antisymmetric K_{ij}^a is absent and so is the bolus velocity, this being the reason why u^* was never found before.

8. CONCLUSIONS

In the Letter, we have discussed five topics. First, the assumption that SGSs are only dissipative is not correct since large scales stir, mix, and dissipate. Second, even if one assumes a dissipation-only model, present LESs still lack the internal consistency check (eq. [7]) that must be satisfied. Third, we have derived an explicit SGS model, equation (2d), that includes dissipation, mixing, and stirring. Fourth, we have provided a turbulence model to compute all the ingredients of the new SGS. Fifth, we have shown that the antisymmetric part of the heat diffusivity contributes to the advection of the SGS model. The new SGS model is given by equations (2c), (2d), (8a)–(8e), (5a), (5b), (6c), and (10a)–(10c). K. L. Chan (2000, private communication) has found that in the new SGS model (eq. [2d]), the advective term is about 50% of the first term (computed with the Smagorinsky model), while the divergence terms are very large (an order of magnitude larger) near the convective-radiative border, while they are small inside the convective zone.

APPENDIX

The explicit form of the Λ-functions, equation (11a), is as follows (C99, eq. [157]):

$$D\Lambda_0 = 1 + \lambda_1 - \lambda_2, \qquad -D\Lambda_1 = 1 + \lambda_1, \qquad D\Lambda_2 = 1, \qquad D = 1 + \lambda_1 - \lambda_2 + \lambda_3, \tag{A1}$$

$$\lambda_1 = \{\mu\}, \qquad -2\lambda_2 = \lambda_1^2 - \{\mu^2\}, \qquad 6\lambda_3 = \lambda_1^3 + 2\{\mu^3\} - 3\lambda_1\{\mu^2\}, \tag{A2}$$

$$\{\mu\} = \mu_{ii}, \qquad \{\mu^2\} = \mu_{ij}\mu_{ji}, \qquad \{\mu^3\} = \mu_{ij}\mu_{jk}\mu_{ki}. \tag{A3}$$

REFERENCES

Canuto, V. M. 1994, ApJ, 428, 729
———. 1997, ApJ, 482, 827 (C97)
———. 1999, ApJ, 524, 311 (C99)
Gille, S. T., & Davis, R. E. 1999, J. Phys. Oceanogr., 29, 1109
Hossain, M., & Mullan, D. J. 1991, ApJ, 380, 631
Kim, Y. C., & Chan, K. L. 1998, ApJ, 496, L121 (KC)
Kimmel, S. J., & Domaradzki, J. A. 2000, Phys. Fluids, 12, 169

Marcus, P. S. 1986, in Astrophysical Radiation Hydrodynamics, ed. K. H. A. Winkler & M. L. Norman (Dordrecht: Reidel), 387
Porter, D. H., & Woodward, P. R. 1994, ApJS, 93, 309
Sofia, S., & Chan, K. L. 1984, ApJ, 282, 550
Stein, R. F., & Nordlund, Å. 1998, ApJ, 499, 914
Xie, X., & Toomre, J. 1991, in Lect. Notes Phys. 388, Challenges to Theories of the Structure of Moderate-Mass Stars, ed. D. O. Gough & J. Toomre (Berlin: Springer), 147